ISST Journal of Applied Physics, Vol. 6 No. 1, (January - June), p.p. 1-10
ISSN No. 0976-903X © Intellectuals Society for Socio-Techno Welfare

RESOLUTION OF AMBIGUITIES AND THE DISCOVERY OF TWO NEW SPACE LATTICES

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MS Received Through : National Conference on Applied Physics and Material Science,
held on February 5-6 2015, at M.D. University, Rohtak, Haryana

ABSTRACT

Based on identical sphere (atom) models, a comprehensive study of SH and HCP has been carried out for the first time by constructing the unit cells (e.g. the conventional, primitive, Wigner–Seitz, reciprocal and Brillouin zone) of HCP and comparing them with their SH counterparts to resolve the existing ambiguities between them. This has been further supported by a comprehensive crystallographic calculation. Similarly, a thorough study of symmetry of the two unit cells has been carried out to decide their positions in the final crystal system table.

The geometrical study suggests the existence of rhombohedral close packing (RCP) and its inherent structural connection with HCP throughout (i.e. as its primitive cell, etc.). Similarly, the study of symmetry suggests the existence of a Trigonal unit cell and its inherent association with SH throughout as a symmetry derivative. The present study resolves clearly that SH, Trigon, HCP and RCP are exclusive and independent lattices where HCP and RCP are exclusively associated with the close packing of identical atoms and hence proposed to be included as independent members of the space lattices. Henceforth, the two new lattices will be called as Wahab lattices (or W lattices) and the sixteen lattices together as Bravais-Wahab lattices (or BW lattices) or simply space lattices as before. The sixteen lattices have been divided into eight crystal systems in the order of their increasing symmetry. The results obtained from the present study help explain the existence of 73 symmorphic space groups in 3-dimensional crystal system. These findings will have immediate as well as far reaching implications.

Keywords: *HCP; RCP; lattice translation, CCP, FCC, Point Group, Space Group, Crystal Systems*

INTRODUCTION

In 1848, Bravais for the first time proposed the concept of 14 space (Bravais) lattices possible in crystalline solids on the basis of primitive translation vectors. However, as compared to simple hexagon (SH) and face centered cubic/ cubic close packing (FCC/CCP), very little crystallographic data for hexagonal close packed (HCP) unit cell as a lattice are available in the existing literature. The words like ambiguity, complexity or confusion are commonly found to exist in literature regarding the representation of hexagonal, trigonal and rhombohedral crystal systems [1–4]. Also, the use of the word primitive for an HCP unit unlike BCC and FCC units is not well understood. These problems have remained unexplained so far.

In the present work, we have developed a new methodology to resolve the existing ambiguities related to SH, Trigon, HCP and RCP and to understand completely the similarities and differences among them. To do so, we initially carried out the geometrical constructions of simple hexagonal (SH) and hexagonal close packed (HCP) units to illustrate their conventional and primitive unit cells and to understand their similarities and differences. For similar reasons then, we constructed their Wigner–Seitz unit cells and Brillouin zones. The primitive unit, the Wigner-Seitz and the Brillouin Zone of HCP are found to have the shapes identical to their FCC/CCP counterparts but with a different orientation. This result is unique and has been observed for the first time. Further, simple crystallographic calculations were made to verify the results obtained from these geometrical constructions. The results obtained for lattice parameters are provided in Table 1 and the volumes of all unit cells in Table 2, respectively.

Similarly, a comprehensive study of symmetries of the two unit cells shows that each; SH (with its ally Trigon) and HCP (with its ally RCP) exhibits 12 independent point groups. Out of the 12 point groups, five belong to SH and seven belong to Trigon, respectively showing 6-fold and 3-fold pure rotational symmetry. Similarly in the other case, seven point groups belong to HCP and five belong to RCP, where all of them show 3-fold pure rotational symmetry. It is interesting to note that Trigonal and HCP unit cells show identical point groups. On the other hand, both SH and RCP unit cells show equal number but different point groups.

The geometrical study clearly suggests that SH and HCP represent independent lattices and not the same. Further, a rhombohedron is found to be the primitive unit of both HCP and CCP units and respectively arrange horizontally and vertically in them. However, only the vertically arranged rhombohedron in CCP along with HCP is the independent lattice exhibited by the close packing of identical atoms. This allows us to conclude that HCP and RCP (henceforth named as Wahab or W lattices) are exclusive and independent lattices and hence should be included in the list of space lattices as independent members to make the total number as 16. They have been suitably divided into 8 crystal systems with increasing order of symmetry. The results obtained from the present study help explain completely the existence of 73 symmorphic space groups in 3-dimensional crystal system (Table 3). These findings will necessarily bring a new era in the understanding of many crystallographic concepts and will have far reaching consequences.

CONSTRUCTION OF SH, HCP AND CCP UNIT CELLS

Let us consider four close packed layers of identical spheres of radius R (in the present case R = 50mm) of A – type as shown in Fig. 1a [4–6]. In the first case, the second layer is placed such that the upper spheres just touch the tips of the lower spheres (so that a=b=c, a special case) to get a simple hexagonal (SH) structure as shown in Fig. 1b (however, in general a=b≠c is a standard consideration for SH structures). On the other hand, by displacing the upper layers properly, we can obtain the HCP and CCP/ FCC structures as shown in Fig. 1. Let us now consider the primitive unit cell (shaded portion) in each case for lattice parameter calculations. In case of SH and CCP/FCC results are only reproduced here for the sake of comparison as these systems are well described in literature.

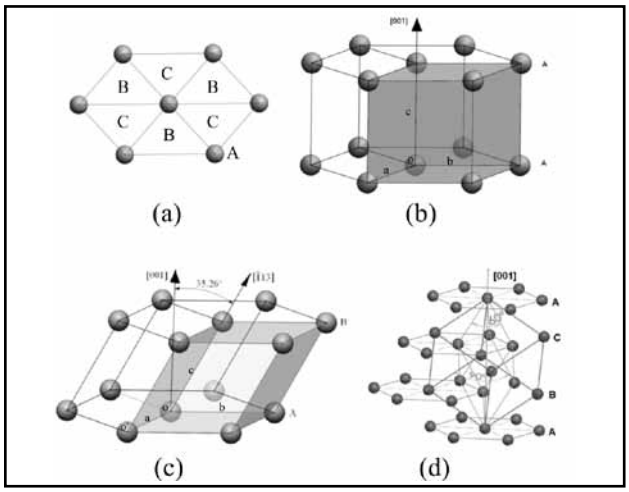

Fig. 1: Packing of identical layers in (a) single layer (b) SH (c) HCP (d) CCP

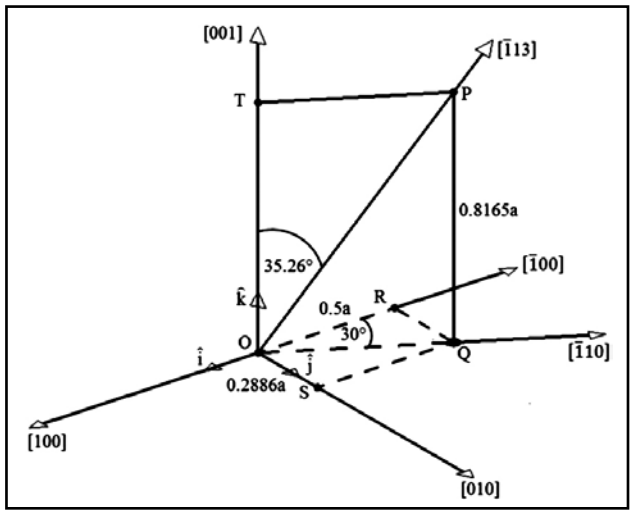

Fig. 2: Spherical polar and Cartesian coordinate system

UNIT CELL CALCULATIONS

Hexagonal Close Packing (HCP)

For the first time, we define the HCP lattice by

$$a = b = c = 2R;\ \alpha = 60°,\ \beta = \gamma = 120°$$

The c–axis changes its direction from [001] in SH to [$\bar{1}$13] in HCP (AB cyclic) unit (Fig. 1c). Let us obtain various lattice parameters.

1. Primitive lattice translations

The translation vectors of the primitive unit cell can be written with the help of spherical polar coordinate system of Fig. 1c shown in Fig. 2. They are obtained for the first time as

$$\vec{a} = a\hat{i},\ \vec{b} = -\frac{a}{2}\hat{i} + \frac{\sqrt{3}a}{2}\hat{j},\ \vec{c} = -\frac{a}{2}\hat{i} + \frac{a}{2\sqrt{3}}\hat{j} + \frac{\sqrt{2}a}{\sqrt{3}}\hat{k} \qquad (1)$$

where $\hat{i}, \hat{j}, \hat{k}$ are unit vectors along the rectangular axes. Magnitude of these vectors is found to be the same, i.e.

$$|\vec{a}| = |\vec{b}| = |\vec{c}| = \vec{a} \qquad (2)$$

The angles between different pair of axes can be determined by using the general equations such as

$$\cos\alpha = \frac{b.c}{|b||c|} = 0, \text{ we obtain } \quad \alpha = 60°,\ \beta = \gamma = 120° \qquad (3)$$

when the origin is at O. This is equivalent to $\alpha = \beta = \gamma = 60°$ if the origin is shifted to O′ (Fig. 1c).

From the above parameters, one can obtain the following quantities:

2. Volume of the primitive unit cell

$$V = a.b\times c = a\hat{i}.\left(-\frac{a}{2}\hat{i}+\frac{\sqrt{3}a}{2}\hat{j}\right)\times$$

$$\left(-\frac{a}{2}\hat{i}+\frac{a}{2\sqrt{3}}\hat{j}+\frac{\sqrt{2}a}{\sqrt{3}}\hat{k}\right)=\frac{a^3}{\sqrt{2}}=$$

$4\sqrt{2}R^3$ (for HCP, a=2R) (4)

Therefore, the volume of HCP unit cell is:

$$V_{HCP} = 3\times 4\sqrt{2}R^3 = 12\sqrt{2}R^3$$

We can obtain the same value of volume (as in eq. 4) by using the lattice parameters given in equations 2 and 3 and substituting them in the standard formula for a rhombohedron, i.e.

$$V = a^3(1 - 3\cos^2\alpha + 2\cos^3\alpha)^{1/2}$$

The crystallographic data obtained from equations 2–4, confirm that the primitive unit cell shown in Fig. 1c is a close packed rhombohedron (RCP) and in general, its axial parameters are written as

$$a = b = c; \qquad \alpha = \beta = \gamma = 60° \tag{5}$$

3. The reciprocal lattice translations

$$a^*=2\pi\frac{b\times c}{a.b\times c}=\frac{2\pi}{a}\left(\hat{i}+\frac{1}{\sqrt{3}}\hat{j}+\frac{1}{\sqrt{6}}\hat{k}\right),$$

$$b^*=\frac{2\pi}{a}\left(\frac{2}{\sqrt{3}}\hat{j}-\frac{1}{\sqrt{6}}\hat{k}\right),\ c^*=\frac{2\pi}{a}\left(\frac{\sqrt{3}}{\sqrt{2}}\hat{k}\right)$$

This gives us

$$\left|a^*\right|=\left|b^*\right|=\left|c^*\right|=\frac{\sqrt{3}}{\sqrt{2}}\left(\frac{2\pi}{a}\right) \tag{6}$$

4. Volume of the reciprocal unit cell

$$V_{RCP} = a^*.b^*\times C^* = \sqrt{2}\left(\frac{2\pi}{a}\right)^3 = \frac{1}{4\sqrt{2}}\left(\frac{2\pi}{R}\right)^3 \tag{7}$$

(for RCP, a = 2R)

Equations 4 and 7 are reciprocal of each other.

5. Angles between reciprocal lattice translations

The calculation of angles as above, gives us:

$$\alpha^* = 109.47°, \beta^* = \gamma^* = 70.53° \tag{8}$$

Simple Hexagon (SH)

The primitive translation vectors of simple hexagonal unit cell with a = b = c = 2R, α = β = 90° and γ = 120° can be found in standard text [4–5]. Also considering Fig. 1b, they are obtained as:

$$\vec{a} = a\hat{i}, \vec{b} = -\frac{a}{2}\hat{i}+\frac{\sqrt{3a}}{2}\hat{j}, \vec{c} = a\hat{k}$$

The magnitude of translation vectors are:

$$\left|\vec{a}\right| = \left|\vec{b}\right| = \left|\vec{c}\right| = \vec{a}$$

The angles between the pair of axes are: α = β = 90° and γ = 120°

From the given parameters, one can obtain the following quantities:

1. Volume of the primitive unit cell

$$V = a.b\times c = a\hat{i}\left(-\frac{a}{2}\hat{i}+\frac{\sqrt{3a}}{2}\hat{j}\right)\times a\hat{k} =$$

$$\frac{\sqrt{3a^3}}{2} = 4\sqrt{3R^3} \quad (\text{for SH}, a = 2R)$$

Therefore, the volume of the hexagonal unit cell is

$$V_{SH} = 3\times 4\sqrt{3}R^3 = 12\sqrt{3}R^3$$

2. The reciprocal lattice translations

$$a^* = 2\pi\frac{b\times c}{a.b\times c}=\frac{2\pi}{a}\left(\hat{i}+\frac{a}{\sqrt{3}}\hat{j}\right), b^* = 2\pi\frac{c\times a}{a.b\times c} =$$

$$\frac{2\pi}{a}\left(\frac{2}{\sqrt{3}}\hat{j}\right), c^* = 2\pi\frac{a\times b}{a.b\times c}=\frac{2\pi}{a}\left(\hat{k}\right)$$

This gives us

$$\left|a^*\right|=\left|b^*\right|=\frac{2}{\sqrt{3}}\left(\frac{2\pi}{a}\right)\text{and}\left|c^*\right|=\frac{2\pi}{a}\Rightarrow\left|a^*\right|=\left|b^*\right|\neq\left|c^*\right|$$

3. Volume of the reciprocal unit cell

$$V^*_{SH} = a^*.b^*\times c^* = \frac{2\pi}{a}\left(\hat{i}+\frac{1}{\sqrt{3}}\hat{j}\right).\frac{2\pi}{a}\left(\frac{2}{\sqrt{3}}\hat{j}\right)\times\frac{2\pi}{a}\hat{k} =$$

$$\frac{2}{\sqrt{3}}\left(\frac{2\pi}{a}\right)^3 = \frac{1}{4\sqrt{3}}\left(\frac{2\pi}{R}\right)^3 \text{ (for SH, a = 2R)}$$

4. Angles between reciprocal lattice translations are:
$\alpha^* = 90°$, $\beta^* = 90°$ and $\gamma^* = 60°$

This implies that the reciprocal lattice is also hexagonal except that it is rotated w.r.t. the direct lattice through an angle of 30° [4].

Face Centered Cubic (FCC)
The crystallographic data of FCC/CCP is very well established. They are:

1. Primitive lattice translations

$$a' = \frac{a}{2}\left(\hat{i}+\hat{j}\right)\ \ b' = \frac{a}{2}\left(\hat{j}+\hat{k}\right)\ c' = \frac{a}{2}\left(\hat{k}+\hat{i}\right)$$

where, a is the side of the conventional unit cube. This gives us

$$|a'| = |b'| = |c'| = a';\quad \alpha' = \beta' = \gamma' = 60° \tag{9}$$

The above crystallographic data in eq. 9 suggests that the primitive unit of FCC/CCP similar to the primitive unit of HCP (eq. 5) is a rhombohedron (close packed).

2. Volume of the primitive cell

$$V = a'.b' \times c' = \frac{a^3}{4} = 4\sqrt{2R^3}\quad (\text{for FCC/CCP}, \sqrt{2}a = 4R) \tag{10}$$

Comparing equations 4 and 10, we observe that the volumes of the two rhombohedrons, i.e. the primitive units of HCP and FCC/CCP are equal. However, their orientations are found to be different as illustrated in Fig. 1. In an HCP, the primitive rhombohedral cells are arranged in horizontal manner and three of them together form a single HCP unit. On the other hand, in CCP they are arranged vertically and represent the same ABC… sequence in the structure (volume wise, a CCP unit is equivalent to four rhombohedral units). It is important to mention here that it is the vertically arranged rhombohedron which represents the independent unit cell and hence independent lattice. Thus according to Fig. 1d, the smallest rhombohedral structure is 3R.

3. Primitive translation vectors a*, b*, c* of the reciprocal lattice

$$a^* = \frac{2\pi}{a}\left(\hat{i}+\hat{j}-\hat{k}\right)\quad b^* = \frac{2\pi}{a}\left(-\hat{i}+\hat{j}+\hat{k}\right)\quad c^* = \frac{2\pi}{a}\left(\hat{i}-\hat{j}+\hat{k}\right)$$

$$\text{where, } |a^*| = |b^*| = |c^*| = \sqrt{3}\left(\frac{2\pi}{a}\right) = \frac{\sqrt{3}}{\sqrt{2}}\left(\frac{2\pi}{a'}\right)$$

$$(\text{for FCC } a = \sqrt{2}a' \text{ and } a' = 2R) \tag{11}$$

4. Volume of the resulting (reciprocal) primitive cell

$$V^* = a^*.b^* \times c^* = 4\left(\frac{2\pi}{a}\right)^3 = \frac{1}{4\sqrt{2}}\left(\frac{2\pi}{R}\right)^3 \tag{12}$$

(for FCC, $\sqrt{2}a = 4R$)

Comparing equations 7 and 12, the reciprocal unit cell volumes in terms of radius R of the sphere corresponding to HCP and FCC/CCP are found to be equal.

5. Angles between the reciprocal lattice translations are:

$$\alpha^* = \beta^* = \gamma^* = 109.47° \tag{13}$$

Equations 8 and 13 indicate that the angles between the axes of reciprocal units corresponding to HCP and CCP are different although their primitive units are identical in shape and volume.

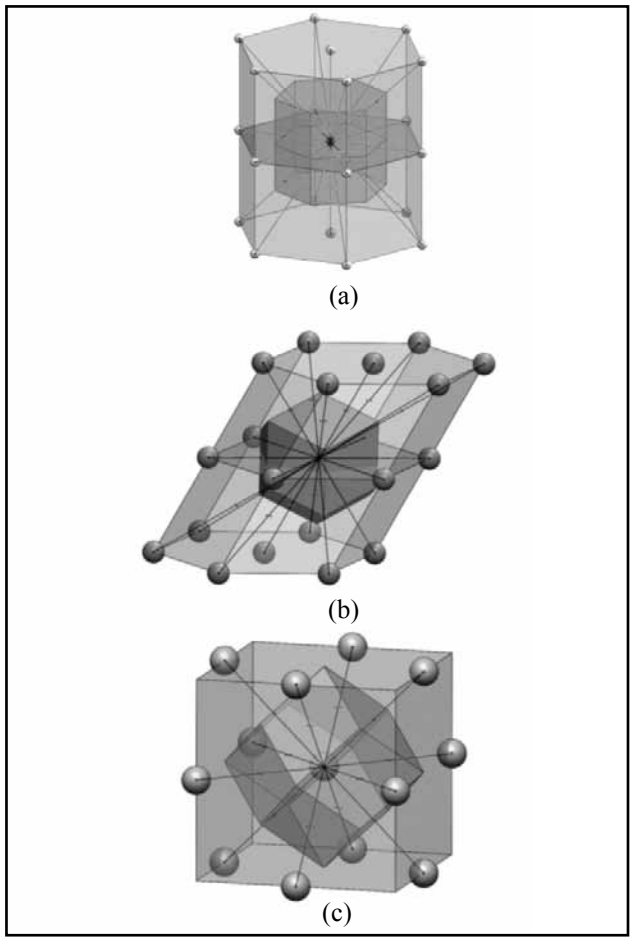

Fig. 3: The Wigner–Seitz unit cell for (a) SH, (b) HCP and (c) FCC

Construction of Wigner–Seitz unit cells of SH, HCP and FCC

Wigner–Seitz unit cells were constructed for SH, HCP and FCC structures following the standard procedure described in a text book [6]. Their final figures are shown in Fig. 3. The resulting Wigner–Seitz unit cell shape of SH is a hexagon and that of HCP and FCC is a rhombic dodecahedron (with a difference in their orientation). As we know that the volume of Wigner–Sietz unit cell is equal to the primitive unit cell volume of the corresponding conventional unit cell. Therefore, the volumes of the corresponding Wigner–Seitz unit cell are

$$(V_{WS})_{SH} = \frac{2 \times V_{SH}}{6} = \frac{V_{SH}}{3} = \frac{12\sqrt{3}R^3}{3} = 4\sqrt{3}R^3$$

$$(V_{WS})_{HCP} = \frac{2 \times V_{HCP}}{6} = \frac{V_{HCP}}{3} = \frac{12\sqrt{2}R^3}{3} = 4\sqrt{2}R^3 = (V_{WS})_{FCC}$$

Construction of Brillouin Zones of SH, HCP and FCC

By definition, a Brillouin Zone is the Wigner–Sietz unit cell of a reciprocal lattice of the given crystal system. Based on

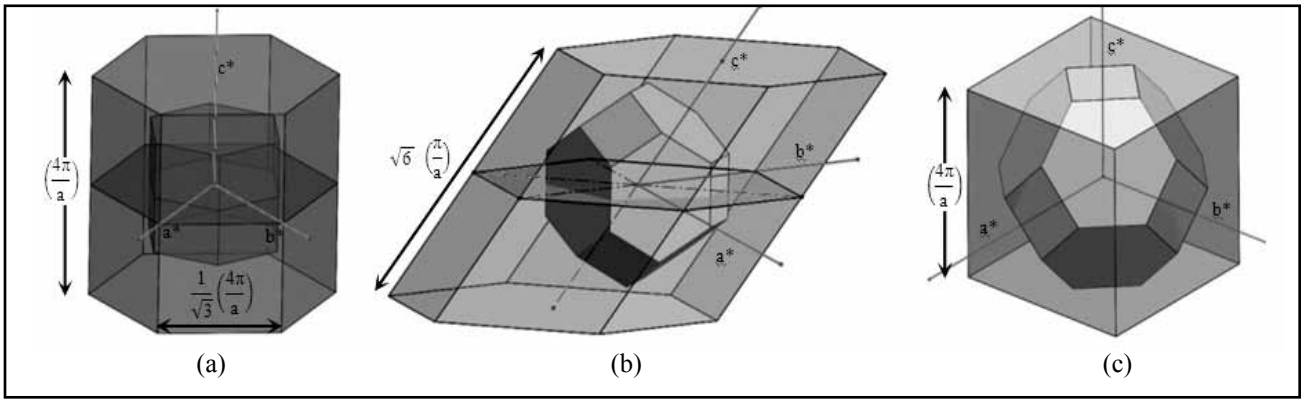

Fig. 4. The Brillouin Zones for (a) SH, (b) HCP and (c) FCC

this principle, Brillouin Zones were constructed for SH, HCP and FCC structures. They are shown in Fig. 4. The resulting BZ shape of SH remains a hexagon and that of HCP and FCC/CCP a cubo–octahedron, respectively. However, just like the Wigner–Seitz cells of HCP and FCC/CCP, their BZ's are also identical in shape and volume. A brief summary of the axes and volumes of the three unit cells are provided in Table 1 and 2, respectively.

Table-1: Comparison of unit cell shape and axes for SH, HCP and FCC/CCP lattices

Lattice type	Direct Lattice		Reciprocal Lattice	
	Primitive Lattice	Wigner–Sietz Unit Cell	Reciprocal Lattice	Brillouin Zone
SH (special) a = b = c = 2R α = β = 90°, γ = 120°	SH a = b = c = 2R	SH	SH a* = b* ≠ c* Axes (x and y) rotate thorough 30°	SH
HCP a = b = c = 2R α = 60°, β = γ = 120°	RCP a = b = c = 2R α = β = γ = 60°	Rhombic Dodecahedron	Trigonal $a^* = b^* = c^* = \frac{\sqrt{3}}{\sqrt{2}}\left(\frac{2\pi}{a}\right)$ α* = 109.47°, β* = γ* = 70.53°	Truncated octahedron
FCC/CCP a = b = c α = β = γ = 90°	RCP a' = b' = c' = 2R α = β = γ = 60°	Rhombic Dodecahedron	Trigonal $a^* = b^* = c^* = \frac{\sqrt{3}}{\sqrt{2}}\left(\frac{2\pi}{a'}\right)$ α* = β* = γ* = 109.47°	Truncated octahedron

Table-2: Comparison of unit cell volumes for SH, HCP and FCC/CCP

Lattice type	Direct Lattice			Reciprocal Lattice	
	Conventional Lattice	Primitive Lattice	Wigner–Sietz Unit Cell*	Reciprocal Lattice	Brillouin Zone*
SH	$12\sqrt{3}R^3$	$4\sqrt{3}R^3$	$4\sqrt{3}R^3$	$\frac{1}{4\sqrt{3}}\left(\frac{2\pi}{R}\right)^3$	$\frac{1}{4\sqrt{3}}\left(\frac{2\pi}{R}\right)^3$
HCP	$12\sqrt{2}R^3$	$4\sqrt{2}R^3$	$4\sqrt{2}R^3$	$\frac{1}{4\sqrt{2}}\left(\frac{2\pi}{R}\right)^3$	$\frac{1}{4\sqrt{2}}\left(\frac{2\pi}{R}\right)^3$
FCC/CCP	$16\sqrt{2}R^3$	$4\sqrt{2}R^3$	$4\sqrt{2}R^3$	$\frac{1}{4\sqrt{2}}\left(\frac{2\pi}{R}\right)^3$	$\frac{1}{4\sqrt{2}}\left(\frac{2\pi}{R}\right)^3$

For rhombic dodecahedron, $\frac{\ell}{R}=\frac{\sqrt{3}}{\sqrt{2}}$ for truncated octahedron, $\frac{\ell}{R}=\frac{\sqrt{2}}{\sqrt{3}}$ (where *l* is the side of the polyhedron)

Study of SH and HCP unit cell symmetries

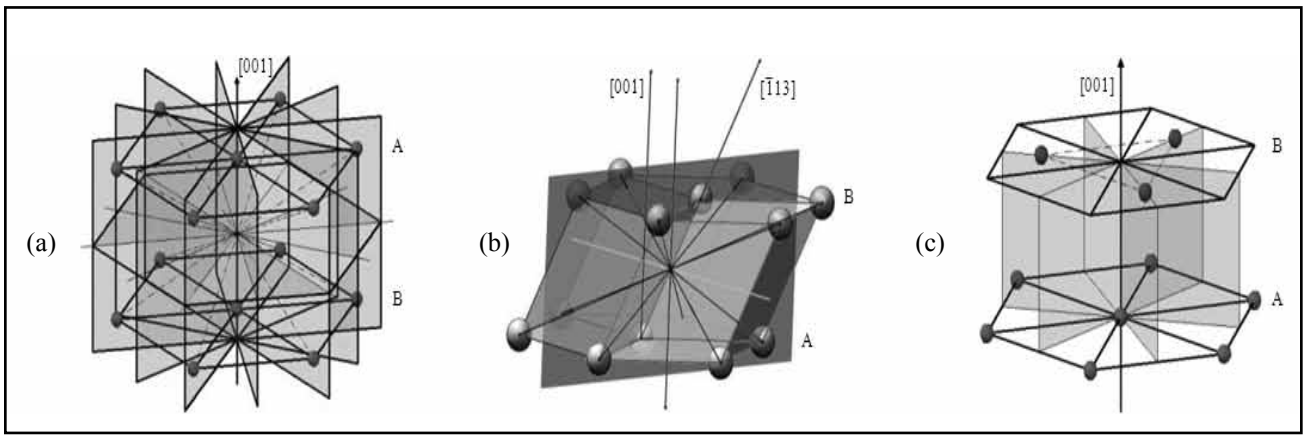

Fig. 5: Fig. 5. Symmetries exhibited by (a) SH unit cell, (b) and (c) HCP unit cell

Let us begin with a single HCP (layer) plane as shown in Fig. 1a, whose maximum symmetry is 6mm. The symmetries of SH and HCP unit cells are found to be different as shown in Fig. 5, where (a) shows full symmetries of SH unit and (b) and (c) show the symmetries of HCP unit w.r.t the tilted axis (a center of symmetry and one vertical mirror) and the principal axis (3-fold proper rotation and three vertical mirrors), respectively. However, for the sake of comparison with SH, we have to consider the symmetries w.r.t the principal axis of HCP unit only (i.e. Fig. 5c).

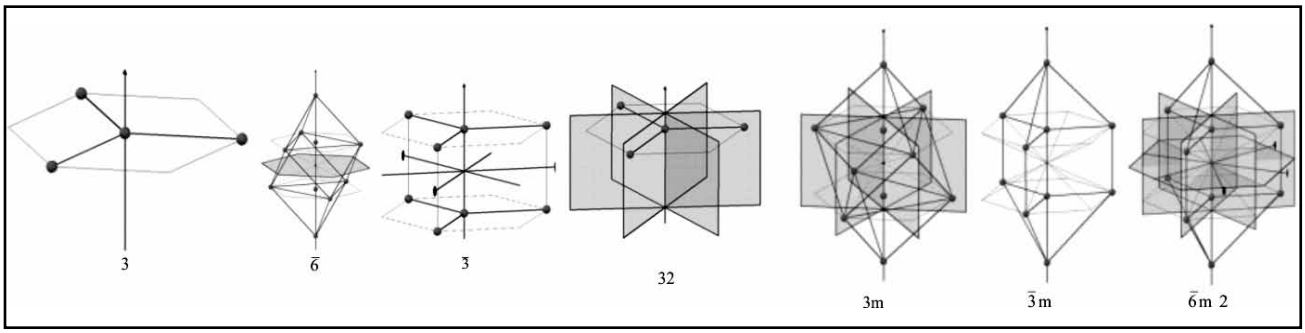

Fig. 6. Illustration of Trigonal point groups

Working out all possible cases, we can obtain 12 point groups under each category. Out of the first 12 point groups, seven (i.e. 3, $\bar{6}$, $\bar{3}$, 32, 3m, $\bar{3}$m and $\bar{6}$m2) show 3-fold while five (i.e. 6, 6/m, 622, 6mm and 6/mmm) show 6-fold proper rotational symmetries, respectively. Hence, they respectively should belong to trigonal (Fig. 6) and hexagonal (Fig. 7) crystal systems. It is important to mention that through literature survey [9] we have come to know that the point groups $\bar{6}$ and $\bar{6}$m2 were a part of trigonal crystal system initially but later on shifted to hexagonal crystal system because of some reasons. Therefore, based on the symmetry considerations (this is clear from Schoenflies notation used in Table 3) they must be shifted back to their original right place.

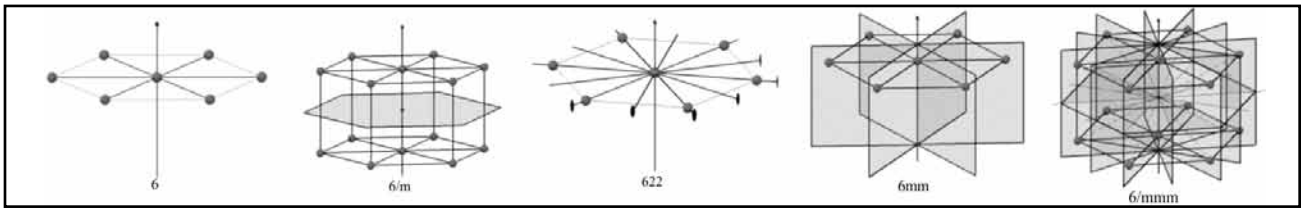

Fig. 7: Illustration of SH point groups

Similarly, out of the second set of 12 point groups exhibited by the close packed structures made of identical atoms, seven show trigonal symmetry (these point groups are identical to the trigonal case) and five rhombohedral symmetry. Thus, seven point groups belong to HCP (Fig. 8) and five belong to RCP (Fig. 9), as illustrated in respective diagrams. It is interesting to see that the trigonal and HCP crystal systems share identical point groups and therefore both of them should be placed in the same crystal system. On the other hand, the simple hexagonal and rhombohedral (close packed) crystal systems have the same number but possess different point groups and therefore they should be under separate crystal system. A revised data for the crystal systems and point groups are provided in Table 3.

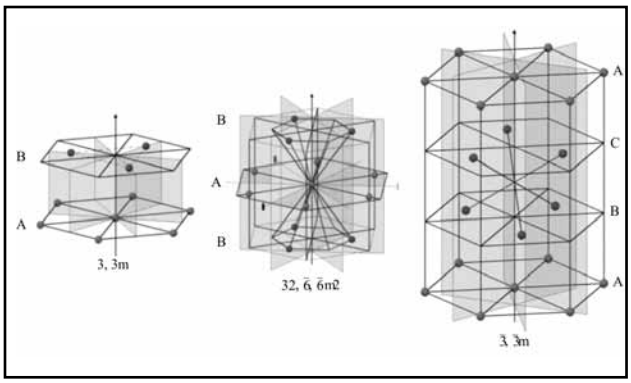

Fig. 8: Illustration of HCP point groups

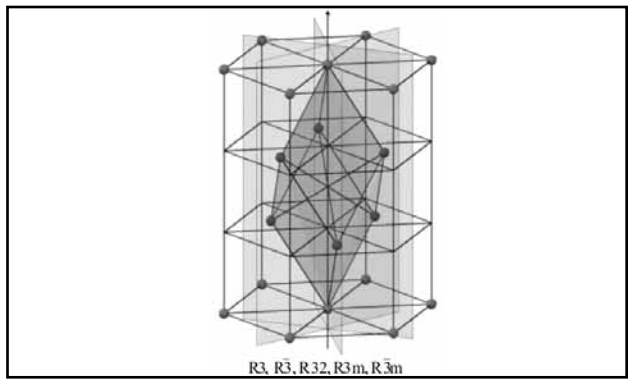

Fig. 9: Illustration of rhombohedral

Table-3: Revised Data of Crystal Systems and Point Groups

Crystal System	Point Groups Notations			
	Herman Mauguin (International)		Schoenflies	
	Non-Centrosymmetric	Centrosymmetric	Non-Centrosymmetric	Centrosymmetric
Triclinic	1	$\bar{1}$	C_1	C_i
Monoclinic	2, m	$^2/_m$	C_2, C_s	C_{2h}
Orthorhombic	222, mm2	mmm	D_2, C_{2v}	D_{2h}
Rhombohedral (CP)*	3 32, 3m	$\bar{3}$ $\bar{3}$m	C_3 D_3, C_{3v}	C_{3i} D_{3d}
Trigonal Hexagonal (CP)*	3, $\bar{6}$ 32, 3m, $\bar{6}$m2	$\bar{3}$ $\bar{3}$m	C_3, C_{3h} D_3, C_{3v}, D_{3h}	C_{3i} D_{3d}

Tetragonal	$4, \bar{4}$ $422, 4mm, \bar{4}2m$	$4/m$ $4/mmm$	C_4, S_4 D_4, C_{4v}, D_{2d}	C_{4h} D_{4h}
Simple Hexagonal	6 622, 6mm	$6/m$ $6/mmm$	C_6 D_6, C_{6v}	C_{6h} D_{6h}
Cubic	23 $432, \bar{4}3m$	$m\bar{3}$ $m\bar{3}m$	T O, T_d	T_h O_h

* CP stands for close packing

Derivation of Symmorphic space groups

Literature survey reveals that there exist 73 symmorphic space groups for 3D crystal systems. However, on using the formula: Symmorphic space group = No. of lattices × No. of point groups, we can obtain only 61 (12 short) corresponding to 14 space lattices. The crystal system, the point groups and the number of symmorphic space groups for 3D, are provided in Table 4.

Important Results

Important results obtained from the comparison of SH and HCP unit cells are:

1. A simple hexagonal lattice (SH) is well known and defined as $a = b = c = 2R$, $\alpha = \beta = 90°$ and $\gamma = 120°$, while a hexagonal close packed (HCP) lattice is defined for the first time with
   $a = b = c = 2R$, and $\alpha = 60°$, $\beta = \gamma = 120°$
2. One SH unit is made up of three parallelepiped units, while one HCP unit is made up of three rhombohedral close packed (RCP) units. That is, the primitive unit of SH remains SH, while the primitive unit of HCP is RCP. In both cases, three primitive units are completely contained within their respective unit cells.
3. The axis of the simple hexagonal unit is the same as the principal axis, i.e. along [001] direction, while the axis of cyclic AB unit of HCP is along $[\bar{1}13]$ direction,
   i.e. $\cos^{-1}\left(\frac{\sqrt{2}}{\sqrt{3}}\right) = 35.26°$ away from the principal axis.
4. Both, the constructions as well as calculations of Wigner–Seitz units and the Brillouin Zones corresponding to two unit cells (SH and HCP) suggest that the resulting shape for SH remains simple hexagonal, while for HCP they are rhombic dodecahedron and truncated octahedron, respectively (Table 2).
5. The study of symmetry related to SH and HCP suggests that a simple hexagonal structure must have a 6-fold pure rotation, trigon and HCP must have a $3, \bar{3}$ or $\bar{6}$-fold rotation while a rhombohedral structure must have a 3 or $\bar{3}$-fold rotation, where a trigonal structure is non close packed but HCP and RCP are close packed.
6. From symmetry point of view, the symmetry elements belonging to trigonal/HCP crystal system remain subgroup of the symmetry elements of simple hexagonal system, while symmetry elements under rhombohedral system remain subgroup of all three, i.e. trigonal/HCP and simple hexagonal.
7. In HCP, the primitive rhombohedral cells are arranged in horizontal manner (Fig. 1b), while in CCP they are arranged vertically (Fig. 1d).
8. In Wigner-Seitz units, the twelve identical bonds of HCP follow 3:6:3 configurations involving three planes of atoms, while in FCC they follow 4:4:4 configurations in three planes of atoms. On the other hand, in Brillouin Zone of HCP, the four hexagonal axes pass through the hexagonal faces of the truncated octahedron, while in the Brillouin Zone of FCC, the three cubic axes pass through the square faces of the truncated octahedron. They are so because the arrangement of atoms in HCP and CCP/FCC are different (Fig. 10).

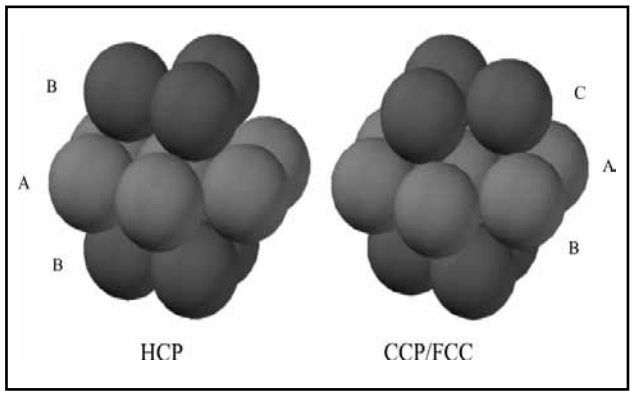

Fig. 10: Arrangement of atoms in HCP and CCP/FCC

9. Both the rhombohedral and cubic units have the identical ABC…sequence in the close packing of polytypic elements and compounds [10]. Actually, from Fig. 1d, the cubic unit can be considered as the second order (three layered) rhombohedron.

10. A number of close packed elements (such as Si, Ge, etc.), MX-compounds (such as SiC, ZnS, etc.) MX_2-compounds (such as CdI_2, PbI_2, etc.) and others exhibit both hexagonal close packed (HCP) and rhombohedral close packed (RCP) structures independently in large numbers, called polytypes [10]. Literature is full of such data.

Table-4: Seventy-Three 3D Symmorphic Space Groups

Crystal System	Lattice Type	Point Groups	Symmorphic Space Groups
Triclinic	P	1, $\bar{1}$	P1, P$\bar{1}$
Monoclinic	P B or C	2, m, $\frac{2}{m}$	P2, Pm, $\frac{P2}{m}$ B2, Bm, $\frac{B2}{m}$
Orthorhombic	P C, A or B I F	222 mm2 mmm	P222, Pmm2, Pmmm C222, Cmm2, Cmmm I222, Imm2, Immm F222, Fmm2, Fmmm
Rhombohedral (CP)	P(RCP)	3, $\bar{3}$, 32, 3m, $\bar{3}$m	R3, R$\bar{3}$, R32, R3m, R$\bar{3}$m
Trigonal Hexagonal (CP)	P HCP	3, $\bar{3}$, 32, 3m, $\bar{3}$m, $\bar{6}$, $\bar{6}$2m	P3, P$\bar{3}$, P32, P3m, P$\bar{3}$m, P$\bar{6}$, P$\bar{6}$2m CP3, CP$\bar{3}$, CP32, CP3m, CP$\bar{3}$m, CP$\bar{6}$, CP$\bar{6}$2m
Tetragonal	P I	4, $\bar{4}$, $\frac{4}{m}$, 422, 4mm, $\bar{4}$2m, $\frac{4}{mmm}$	P4, P$\bar{4}$, $\frac{P4}{m}$, P422, P4mm, P$\bar{4}$2m, $\frac{P4}{mmm}$ I4, P$\bar{4}$, $\frac{I4}{m}$, I422, I4mm, I$\bar{4}$2m, $\frac{I4}{mmm}$
Simple Hexagonal	P	6, $\frac{6}{m}$, 622, 6mm, $\frac{6}{mmm}$	P6, $\frac{P6}{m}$, P622, P6mm, $\frac{P6}{mmm}$
Cubic	P I F	23, m3, 432, $\bar{4}$3m, m3m	P23, Pm3, P432, P$\bar{4}$3m, Pm3m I23, Im3, I432, I$\bar{4}$3m, Im3m F23, Fm3, F432, F$\bar{4}$3m, Fm3m

CONCLUSIONS

The above crystallographic results obtained from the study of identical atoms help us to make the following important conclusions:

1. SH and HCP are found to have no geometrical similarities (i.e. in terms of primitive cell, WS, RL and BZ) and hence they represent different lattices (Tables 1 and 2).

2. RCP is found to be the primitive unit of both HCP and CCP/FCC, inherently related to both and represents an independent form of close packing of identical atoms.

3. SH and HCP retain their own characters both in direct and reciprocal space, while FCC and BCC change into one another in similar situations.

4. Polytypic elements and compounds exhibit both HCP (hexagonal) and RCP (rhombohedral) structures of different periodicity independently (literature survey) and hence must be treated as independent lattices.

5. Since RCP and CCP (is the second order rhombohedron) are represented by the same ABC… sequence, therefore the term RCP should be used instead of CCP to remove any confusion between CCP and FCC.

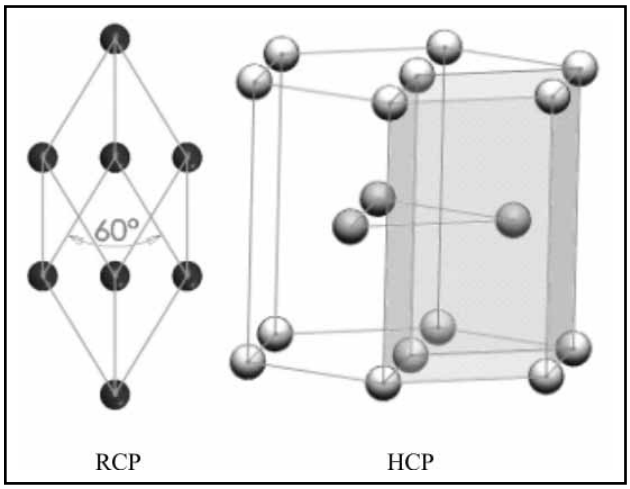

Fig. 11: Showing RCP and HCP lattices

6. Based on unit cell constructions, unit cell calculations and symmetry analyses, the numbers of crystal system in 3-D turn out to be 8.

7. Based on the above findings, we propose that RCP and HCP (Fig. 11) should be added in the list of space lattices as independent members to make the total number as 16. The two new lattices should henceforth be known as Wahab lattices (or W lattices).

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